Inverse design of nanoporous crystalline reticular materials with deep generative models

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Abstract

Reticular frameworks are crystalline porous materials that form via the self-assembly of molecular building blocks in different topologies, with many having desirable properties for gas storage, separation, catalysis, biomedical applications and so on. The notable variety of building blocks makes reticular chemistry both promising and challenging for prospective materials design. Here we propose an automated nanoporous materials discovery platform powered by a supramolecular variational autoencoder for the generative design of reticular materials. We demonstrate the automated design process with a class of metal–organic framework (MOF) structures and the goal of separating carbon dioxide from natural gas or flue gas. Our model shows high fidelity in capturing MOF structural features. We show that the autoencoder has a promising optimization capability when jointly trained with multiple top adsorbent candidates identified for superior gas separation. MOFs discovered here are strongly competitive against some of the best-performing MOFs/zeolites ever reported. Reticular frameworks are crystalline porous materials with desirable properties such as gas separation, but their large design space presents a challenge. An automated nanoporous materials discovery platform powered by a supramolecular variational autoencoder can efficiently explore this space.